Phase space geometry and invariant manifolds underlying reaction dynamics

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Bibliography

[Arn76] V. I. Arnold. *Les méthodes mathématiques de la mécanique classique.* Nauka, Moscow, Éditions Mir, 1976.

[BGH85] J. Binney, O. E. Gerhard, and P. Hut. Structure of surfaces of section. *Mon. Not. R. Astr. Soc.*, 215(1):59–65, 1985.

[Bir27] G. D. Birkhoff. *Dynamical Systems.* AMS, 1927.

[Bow14] J. M. Bowman. Roaming radicals. *Mol. Phys.*, 112(19):2516–2528, 2014.

[BS11] J. M. Bowman and B. C. Shepler. Roaming radicals. *Annu. Rev. Phys. Chem.*, 62:531–553, 2011.

[Che86] W. J. Chesnavich. Multiple transition states in unimolecular reactions. *J. Chem. Phys.*, 84(5):2615–2619, 1986.

[CHM75] S. Chapman, S. M. Hornstein, and W. H. Miller. Accuracy of transition state theory for the threshold of chemical reactions with activation energy. Collinear and three-dimensional $H + H_2$. *J. Am. Chem. Soc.*, 97(4):892–894, 1975.

[Con68] C. C. Conley. Low energy transit orbits in the restricted three-body problem. *SIAM J. Appl. Math.*, 16:732–746, 1968.

[CSB80] W. J. Chesnavich, T. Su, and M. T. Bowers. Collisions in a noncentral field: A variational and trajectory investigation of ion-dipole capture. *J. Chem. Phys.*, 72(4):2641, 1980.

[Dav87] M. J. Davis. Phase space dynamics of bimolecular reactions and the breakdown of transition state theory. *J. Chem. Phys.*, 86(7):3978–4003, 1987.

[EW91] B. Eckhardt and D. Wintgen. Indices in classical mechanics. *J. Phys. A*, 24(18):4335, 1991.

[Fen71] N. Fenichel. Persistence and smoothness of invariant manifolds for flows. *Indiana Univ. Math. J.*, 21:193–226, 1971.

[Gre68] J. M. Greene. Two-dimensional measure-preserving mappings. *Journal of Mathematical Physics*, 9(5):760–768, 1968.

[HCB16] P. L. Huston, R. Conte, and J. M. Bowman. Roaming under the microscope: Trajectory study of formaldehyde dissociation. *J. Phys. Chem. A*, 120:5103–5114, 2016.

[Hen82] J. Henrard. Capture into resonance: An extension of the use of adiabatic invariants. *Celestial mechanics*, 27(1):3–22, 1982.

[Hil05] G. W. Hill. *Collected Mathematical Works of G. W. Hill, vol. 1.* Washington:Carnegie Institute, 1905.

[Hor38] J. Horiuti. On the statistical mechanical treatment of the absolute rate of chemical reaction. *Bull. Chem. Soc. Jpn.*, 13(1):210–216, 1938.

[HPS77] M. W. Hirsch, C. C. Pugh, and M. Shub. *Invariant Manifolds.* Lecture Notes in Mathematics. Springer-Verlag Berlin Heidelberg, 1977.

[HSD04] M. W. Hirsch, S. Smale, and R. L. Devaney. *Differential Equations, Dynamical Systems, and an Introduction to Chaos.* Elsevier, 2004.

[InPS11] M. Iñarrea, A. I. Palacián, J. F.and Pascual, and J. P. Salas. Bifurcations of dividing surfaces in chemical reactions. *J. Chem. Phys.*, 135(1):014110, 2011.

[JFU99] C. Jaffé, D. Farrelly, and T. Uzer. Transition state in atomic physics. *Phys. Rev. A*, 60(5):3833, 1999.

[JRL+02] C. Jaffé, S. D. Ross, M. W. Lo, J. Marsden, D. Farrelly, and T. Uzer. Statistical theory of asteroid escape rates. *Phys. Rev. Lett.*, 89:011101, 2002.

[JSG91] M. J. T. Jordan, S. C. Smith, and R. G. Gilbert. Variational transition state theory: A simple model for dissociation and recombination reactions of small species. *J. Phys. Chem.*, 95(22):8685–8694, 1991.

[Kec67] J. C. Keck. Variational theory of reaction rates. *Adv. Chem. Phys.*, 13:85, 1967.

[Mac90] R. S. MacKay. Flux over a saddle. *Phys. Lett. A*, 145(8,9):425–427, 1990.

[MCE+85] J. D. Meiss, J. R. Cary, D. F. Escande, R. S. MacKay, I. C. Percival, and J. L. Tennyson. Dynamical theory of anomalous particle transport. *Plasma Physics and Controlled Nuclear Fusion Research 1984 Vol.3*, pages 441–448, 1985.

[MCE+14a] F. A. L. Mauguière, P. Collins, G. S. Ezra, S. C. Farantos, and S. Wiggins. Multiple transition states and roaming in ion–molecule reactions: A phase space perspective. *Chem. Phys. Lett.*, 592:282–287, 2014.

[MCE+14b] F. A. L. Mauguière, P. Collins, G. S. Ezra, S. C. Farantos, and S. Wiggins. Roaming dynamics in ion-molecule reactions: Phase space reaction pathways and geometrical interpretation. *J. Chem. Phys.*, 140(13):134112, 2014.

[MCEW13] F. A. L. Mauguière, P. Collins, G. S. Ezra, and S. Wiggins. Bond breaking in a Morse chain under tension: Fragmentation patterns, higher index saddles, and bond healing. *The Journal of Chemical Physics*, 138(13):134118, 2013.

[McG69] R. P. McGehee. Some homoclinic orbits in the restricted three-body problem. *PhD thesis*, 1969.

[MCK+15] F. A. L. Mauguière, P. Collins, Z. C. Kramer, B. K. Carpenter, G. S. Ezra, S. C. Farantos, and S. Wiggins. Phase space structures explain hydrogen atom roaming in formaldehyde decomposition. *J. Phys. Chem. Lett.*, 6(20):4123–4128, 2015.

[MCK+16] F. A. L. Mauguière, P. Collins, Z. C. Kramer, B. K. Carpenter, G. S. Ezra, S. C. Farantos, and S. Wiggins. Phase space barriers and dividing surfaces in the absence of critical points of the potential energy: Application to roaming in ozone. *J. Chem. Phys.*, 144(5):54107, 2016.

[Mei15] J. D. Meiss. Thirty years of turnstiles and transport. *Chaos*, 25(9):097602, 2015.

[Mil76] W. H. Miller. Unified statistical model for “complexÂ´Â´ and “directÂ´Â´ reaction mechanisms. *J. Chem. Phys.*, 65(6):2216–2223, 1976.

[MK71] K. Morokuma and M. Karplus. Collision dynamics and the statistical theories of chemical reactions. ii. Comparison of reaction probabilities. *The Journal of Chemical Physics*, 55(1):63–75, 1971.

[MMP84] R. S. MacKay, J. D. Meiss, and I. C. Percival. Transport in Hamiltonian systems. *Phys. D*, 13(1-2):55–81, 1984.

[MMW98] C. K. McCord, K. R. Meyer, and Q. Wang. The integral manifolds of the three-body problem. *Mem. Amer. Math. Soc.*, 132(628), 1998.

[MS14] R. S. MacKay and D. C. Strub. Bifurcations of transition states: Morse bifurcations. *Nonlinearity*, 27(5):859–895, 2014.

[MS15] R. S. MacKay and D. C. Strub. Morse bifurcations of transition states in bimolecular reactions. *Nonlinearity*, 28(12):4303, 2015.

[OdAdLMM90] A. M. Ozorio de Almeida, N. de Leon, M. A. Mehta, and C. C. Marston. Geometry and dynamics of stable and unstable cylinders in hamiltonian systems. *Physica D*, 46(2):265–285, 1990.

[Ott89] J. M. Ottino. *The Kinematics of Mixing: Stretching, Chaos, and Transport*. Cambridge Texts in Applied Mathematics. Cambridge Univiversity Press, 1989.

[PCP80] P. Pollak, M. S. Child, and P. Pechukas. Classical transition state theory: A lower bound to the reaction probability. *The Journal of Chemical Physics*, 72(3):1669–1678, 1980.

[Pec76a] P. Pechukas. On simple saddle points of a potential surface, the conservation of nuclear symmetry along paths of steepest descent, and the symmetry of transition states. *J. Chem. Phys.*, 64:1516–1521, 1976.

[Pec76b] P. Pechukas. Statistical approximations in collision theory. In H. W. Miller, editor, *Dynamics of Molecular Collisions Part B*, pages 269–322. Plenum Press, 1976.

[Pec81] P. Pechukas. Transition state theory. *Ann. Rev. Phys. Chem.*, 32(1):159–177, 1981.

[PK64] R. N. Porter and M. Karplus. Potential energy surface for H3. *J. Chem. Phys.*, 40(4):1105–1115, 1964.

[PM73] P. Pechukas and F. J. McLafferty. On transition-state theory and the classical mechanics of collinear collisions. *J. Chem. Phys.*, 58:1622–1625, 1973.

[PP78] E. Pollak and P. Pechukas. Transition states, trapped trajectories, and classical bound states embedded in the continuum. *J. Chem. Phys.*, 69(3):1218–1226, 1978.

[PP79a] P. Pechukas and E. Pollak. Classical transition state theory is exact if the transition state is unique. *J. Chem. Phys.*, 71(5):2062–2068, 1979.

[PP79b] E. Pollak and P. Pechukas. Unified statistical model for "complex" and "direct" reaction mechanisms: A test on the collinear H+H2 exchange reaction. *J. Chem. Phys.*, 70(1):325–333, 1979.

[QH84] W. Quapp and D. Heidrich. Analysis of the concept of minimum energy path on the potential energy surface of chemically reacting systems. *Theoret. Chim. Acta (Berl.)*, 66(3):245–260, 1984.

[RKW90] V. Rom-Kedar and S. Wiggins. Transport in two-dimensional maps. *Arch. Ration. Mech. Anal.*, 109(3):239–298, 1990.

[Rui75] O. R. Ruiz. Existence of brake-orbits in Finsler mechanical systems. *PhD thesis*, 1975.

[SA97] K. R. Sreenivasan and R. A. Antonia. The phenomenology of small-scale turbulence. *Annu. Rev. Fluid Mech.*, 29(1):435–472, 1997.

[Sei45] H. Seifert. Periodische Bewegungen mechanischer Systeme. *Math. Z.*, (41):197–216, 1945.

[SK78] D. I. Sverdlik and G. W. Koeppl. An energy limit of transition state theory. *Chem. Phys. Lett.*, 59(3):449–453, 1978.

[Sre91] K. R. Sreenivasan. On local isotropy of passive scalars in turbulent shear flows. *Proc. R. Soc. London. Ser. A*, 434(1890):165–182, 1991.

[TG84] G. D. Truhlar and B. C. Garrett. Variational transition state theory. *Ann. Rev. Phys. Chem.*, 35:159–189, 1984.

[TKK$^+$05] M. Toda, T. Komatsuzaki, T. Konishi, R. S. Berry, and S. A. Rice, editors. *Geometric Structures of Phase Space in Multidimensional Chaos.* John Wiley & Sons, Inc., 2005.

[TLL$^+$04] D. Townsend, A. Lahankar, S. K. Lee, S. D. Chambreau, A. G. Suits, X. Zhang, J. Rheinecker, L. B. Harding, and J. M. Bowman. The roaming atom: Straying from the reaction path in formaldehyde decomposition. *Science*, 306(5699):1158–1161, 2004.

[UJP+02] T. Uzer, C. Jaffé, J. Palacián, P. Yanguas, and S. Wiggins. The geometry of reaction dynamics. *Nonlinearity*, 15:957–992, 2002.

[vZFM93] R. D. van Zee, M. F. Foltz, and C. B. Moore. Evidence for a second molecular channel in the fragmentation of formaldehyde. *J. Chem. Phys.*, 99(3):1664–1673, 1993.

[WBW04a] H. Waalkens, A. Burbanks, and S. Wiggins. A computational procedure to detect a new type of high-dimensional chaotic saddle and its application to the 3D Hill's problem. *J. Phys. A*, 37:L257–L265, 2004.

[WBW04b] H. Waalkens, A. Burbanks, and S. Wiggins. Phase space conduits for reaction in multidimensional systems: HCN isomerization in three dimensions. *J. Chem. Phys.*, 121(13):6207–6225, 2004.

[WBW05a] H. Waalkens, A. Burbanks, and S. Wiggins. Efficient procedure to compute the microcanonical volume of initial conditions that lead to escape trajectories from a multidimensional potential well. *Phys. Rev. Lett.*, 95:084301, 2005.

[WBW05b] H. Waalkens, A. Burbanks, and S. Wiggins. A formula to compute the microcanonical volume of reactive initial conditions in transition state theory. *J. Phys. A*, 38:L759–L768, 2005.

[Wig37] E. Wigner. Calculation of the rate of elementary association reactions. *J. Chem. Phys.*, 5:720–725, 1937.

[Wig38] E. Wigner. The transition state method. *Trans. Faraday Soc.*, 34:29–41, 1938.

[Wig03] S. Wiggins. *Introduction to Applied Nonlinear Dynamical Systems and Chaos*. Springer, New York, 2003.

[Wil36] J. Williamson. On the algebraic problem concerning the normal forms of linear dynamical systems. *American Journal of Mathematics*, 58(1):141–163, 1936.

[WSW08] H. Waalkens, R. Schubert, and S. Wiggins. Wigner's dynamical transition state theory in phase space: classical and quantum. *Nonlinearity*, 21:R1–R118, 2008.

[WW04] H. Waalkens and S. Wiggins. Direct construction of a dividing surface of minimal flux for multi-degree-of-freedom systems that cannot be recrossed. *J. Phys. A*, 37:L435, 2004.

[WW10] H. Waalkens and S. Wiggins. Geometric models of the phase space structures governing reaction dynamics. *Reg. Chaot. Dyn.*, 15:1–39, 2010.

[WWJU01] S. Wiggins, L. Wiesenfeld, C. Jaffé, and T. Uzer. Impenetrable barriers in phase-space. *Phys. Rev. Lett.*, 86:5478–5481, 2001.